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An approach of Finding Second Derivative Finite Differences Compact Schemes

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Abstract:

In solving problems from Computational Fluid Dynamics (CFD) and physics, huge efforts should be afforded to obtain accurate and applicable schemes for the derivatives. Based on the idea of high order polynomials, many sets of second derivative schemes are derived in this paper. These sets are grouped according to the order of the accuracy of the approximations from order three to order seven. Different types of second derivative forward, central, and backward compact with some traditional approximations are introduced at each set by the proposed method. The order of accuracy is verified of each scheme using the technique of finding the values of the coefficients for the error terms by matching both sides of the given scheme. Many schemes that are introduced in this article are applicable to some problems from science and engineering.

Keywords: Compact Scheme, High Order, Finite difference, compact approximation

نهج لايجاد طرق عددية متراسة للمشتقة الثانية

حسن عبد سلمان الدجيلي

قسم الرياضيات ، كلية العلوم، الجامعة المستنصرية، بغداد، العراق

الخلاصة :

لحل مسائل في ديناميكا الموائع الحسابية (CFD) والفيزياء يجب بذل جهود كبيرة للحصول على طرق عددية للمشتقات تكون دقيقة وقابلة للتطبيق. في هذا البحث و بناءاً على فكرة متعددات الحدود عالية الرتبة يتم اشتقاق العديد من مجموعات الطرق العددية للمشتقة الثانية . يتم ترتيب هذه المجموعات وفقاً لرتبة الطرق العددية من الرتبة الثالثة الى الرتبة السابعة. يتم تقديم انواع مختلفة من الطرق العددية (اللامامية , المركزية , والخلفية) المتراسة والاعتيادية للمشتقة الثانية بواسطة المنهجية المقترحة . يتم التحقق من دقة رتبة كل طريقة عددية عن طريق ايجاد معاملات متعددات الحدود المتبقية من خلال مطابقة جهتي الطريقة العددية المعنية . عدد من الطرق العددية التي تم اشتقاقها في هذا البحث قابلة للتطبيق لحل مشكلات من العلوم والهندسة.

1. Introduction:

High order compact numerical algorithms have an essential role to solve problems from engineering and science. Compared to implicit standard finite difference methods, compact

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finite difference methods are explicit and produce high order accuracy with better resolution properties when using the same number of points as verified in [1], [2], and [3]. One approach of finding numerical solution is to use some standard transformations which yields to special types of differential equations, as in [4], [5], and [6]. Because of the importance and the need of the compact finite difference schemes, many intensive studies have been conducted using different approaches. One of the great advantages of the compact schemes is not only finding the first derivative but also higher derivatives as needed in the applications from the Computational Fluid Dynamics (CFD). For example, both first and second derivatives have been evaluated at the same time as discussed in [7] when constructing the combined compact schemes. In [8], high order compact scheme is discussed and constructed according to the analysis of dispersion and dissipation at each stencil and to capture the shock without losing the high resolution of the results. Also, it is not restricted to the uniform grid, many compact schemes of anon-uniform grids have been derived and extended, see [9], [10], and [11] as examples. In [12], the authors introduced a methodology of providing special types of compact schemes by avoiding negative dissipation in some stencils to gain stability and non-oscillatory characteristics. Additionally, efforts were achieved in [13] and [14] to obtain some kinds of compact schemes according to the results from Fourier analysis and applied to different types of continuous and non-continuous problems from CDF. [15] and [16] proposed new families of compact schemes which are applicable to Navier-Stokes equations and to parabolic problems respectively. Recently, new approach of providing high order approximations for the first derivative was proposed in [17] using special kinds of matrices. In this article, six sets of numerical compact schemes for the second derivative are constructed in section 2 by using special kinds of polynomials. In section 3, the orders of accuracy for constructed schemes are confirmed and verified by finding the coefficients of the remaining polynomials or the error terms. Finally, in section 4, conclusions are given.

2. Second Derivative Approach for Approximation:

In this section, approximations for the second derivative are constructed with different orders. A uniform step size $h = x_k - x_{k-1}$ and grid points x_0, x_1, \dots, x_N are used such that $1 \leq k \leq N$. f_k'' represents the approximation of the second derivative of $f(x)$ at x_k such that $f_k = f(x_k)$, $f'_k = f'(x_k)$, and $f''_k = f''(x_k)$. The general form of the second derivative compact finite difference schemes can be expressed as follows:

$$r_1 f''_{k-p} + r_2 f''_{k-p+1} + \dots + r_{m-1} f''_{k-1} + f''_k + r_{m+1} f''_{k+1} + \dots + r_{2m-1} f''_{k+p-1} + r_{2m} f''_{k+p} = \frac{1}{h^2} [s_1 f_{k-p} + s_2 f_{k-p+1} + \dots + s_{m-1} f_{k-1} + s_m f_k + s_{m+1} f_{k+1} + \dots + s_{2m-1} f_{k+p-1} + s_{2m} f_{k+p}]. \quad (1)$$

Usually, The values of the coefficients $r_1, r_2, r_3, \dots, r_{2m}, s_1, s_2, s_3, \dots, s_{2m}$ can be determined using Taylor series expansion at x_k where $1 \leq k \leq N$. In this work, it is assumed that $p = 2$ in Eq.(1), so it follows :

$$r_1 f''_{k-2} + r_2 f''_{k-1} + f''_k + r_4 f''_{k+1} + r_5 f''_{k+2} = \frac{1}{h^2} [s_1 f_{k-2} + s_2 f_{k-1} + s_3 f_k + s_4 f_{k+1} + s_5 f_{k+2}]. \quad (2)$$

Another way of finding the coefficients is using a polynomial of order N

$$T_N(x) = \sum_{t=0}^N c_t x^t \quad (3)$$

such that $T'_N(x) = \sum_{t=1}^N t c_t x^{t-1}$, $T''_N(x) = \sum_{t=2}^N t(t-1) c_t x^{t-2}$.

To derive the schemes in this work, substituting (3) in (2) results in:

$$\begin{aligned}
 & r_1 \sum_{t=2}^N t(t-1)c_t x_{k-2}^{t-2} + r_2 \sum_{t=2}^N t(t-1)c_t x_{k-1}^{t-2} + \sum_{t=2}^N t(t-1)c_t x_k^{t-2} \\
 & + r_4 \sum_{t=2}^N t(t-1)c_t x_{k+1}^{t-2} + r_5 \sum_{t=2}^N t(t-1)c_t x_{k+2}^{t-2} \\
 & = \frac{1}{h^2} \left(s_1 \sum_{t=0}^N c_t (x_{k-2})^t + s_2 \sum_{t=0}^N c_t (x_{k-1})^t + s_3 \sum_{t=0}^N c_t (x_k)^t + s_4 \sum_{t=0}^N c_t (x_{k+1})^t \right. \\
 & \left. + s_5 \sum_{t=0}^N c_t (x_{k+2})^t \right)
 \end{aligned}$$

Now, locating x_k at the origin and assuming that h is equal to one unit lead to:

$$\begin{aligned}
 & \sum_{t=2}^N t(t-1)c_t [r_1(-2)^{t-2} + r_2(-1)^{t-2} + r_4(1)^{t-2} + r_5(2)^{t-2}] + 2c_2 \\
 & = \sum_{t=0}^N c_t [s_1(-2)^t + s_2(-1)^t + s_4(1)^t + s_5(2)^t] + c_0 s_3
 \end{aligned}$$

$$\begin{aligned}
 & \sum_{t=2}^N t(t-1)c_t [r_1(-2)^{t-2} + r_2(-1)^{t-2} + r_4(1)^{t-2} + r_5(2)^{t-2}] + 2c_2 = c_0 [s_1 + s_2 + \\
 & s_3 + s_4 + s_5] + c_1 [-2s_1 - s_2 + s_4 + 2s_5] + \sum_{t=2}^N c_t [s_1(-2)^t + s_2(-1)^t + s_4(1)^t + \\
 & s_5(2)^t]. \tag{4}
 \end{aligned}$$

To get schemes of order t , the coefficient c_t in the polynomial $T_N(x)$ should be a real number not equal to zero, and $c_w = 0$ for $t < w \leq N$. Hence, different sets according to their orders are established from the third order and up to seventh order by matching both sides of Eq.(4). In general, Eq.(2) can be expressed in the matrix form as follows:

$$AF'' = \frac{1}{h} BF \tag{5}$$

such that

$$F = [f_1 \quad f_2 \quad \dots \quad f_N]^T \quad \text{and} \quad F'' = [f''_1 \quad f''_2 \quad \dots \quad f''_N]^T$$

$$A = \begin{bmatrix} 1 & r_4 & r_5 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & r_1 & r_2 \\ r_2 & 1 & r_4 & r_5 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & r_1 \\ r_1 & r_2 & 1 & r_4 & r_5 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & r_1 & r_2 & 1 & r_4 & r_5 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & r_1 & r_2 & 1 & r_4 & r_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & r_1 & r_2 & 1 & r_4 & r_5 \\ r_5 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & r_1 & r_2 & 1 & r_4 \\ r_4 & r_5 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & r_1 & r_2 & 1 \end{bmatrix}$$

$$B = \begin{bmatrix} s_3 & s_4 & s_5 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & s_1 & s_2 \\ s_2 & s_3 & s_4 & s_5 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & s_1 \\ s_1 & s_2 & s_3 & s_4 & s_5 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & s_1 & s_2 & s_3 & r_4 & r_5 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & s_1 & s_2 & s_3 & s_4 & s_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & s_1 & s_2 & s_3 & s_4 & s_5 \\ s_5 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & s_1 & s_2 & s_3 & s_4 \\ s_4 & s_5 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & s_1 & s_2 & s_3 \end{bmatrix}$$

2.1. Set of second derivative approximations of order 3:

In this part, second derivative compact schemes of the third order are constructed as shown in Table 1. To obtain this set of approximations for the second derivative, c_2 in Eq.(4) should not be zero and $c_3, c_4, c_5, \dots, c_N$ are all zeros. Hence, when matching the coefficients in both sides of Eq.(4), it follows:

$$2c_2[r_1 + r_2 + 1 + r_4 + r_5] = c_0[s_1 + s_2 + s_3 + s_4 + s_5] + c_1[-2s_1 - s_2 + s_4 + 2s_5] + c_2[4s_1 + s_2 + s_4 + 4s_5]. \quad (6)$$

Therefore, this set of approximations should satisfy the following equations:

$$\begin{aligned} [s_1 + s_2 + s_3 + s_4 + s_5] &= 0, \\ [-2s_1 - s_2 + s_4 + 2s_5] &= 0, \\ 2[r_1 + r_2 + 1 + r_4 + r_5] &= 4s_1 + s_2 + s_4 + 4s_5. \end{aligned} \quad (7)$$

Table 1: Set of second derivative approximations of order 3

Schemes	r_1	r_2	r_4	r_5	s_1	s_2	s_3	s_4	s_5
SDO3-1	0	0	0	0	0	1	-2	1	0
SDO3-2	0	$-\frac{1}{2}$	0	0	0	0	$\frac{1}{2}$	-1	$\frac{1}{2}$
SDO3-3	$-\frac{1}{3}$	0	0	0	0	0	$\frac{2}{3}$	$-\frac{4}{3}$	$\frac{2}{3}$
SDO3-4	0	0	0	1	0	0	2	-4	2

All approximations in Table 1 are of order three, and they are named according to the order and the location in the table. For example, the scheme SDO3-1 stands for Second Derivative Order 3 – scheme number 1. Similarly, the schemes of the other sets can be derived as follows.

2.2. Set of second derivative approximations of order 4:

In this section, second derivative compact approximations of order four are derived as illustrated in Table 2. To get this set of schemes for the second derivative, c_3 in Eq.(4) should not be zero and c_4, c_5, \dots, c_N are all zeros. From Eq.(4), and it follows:

$$\begin{aligned} 2c_2[r_1 + r_2 + 1 + r_4 + r_5] + 6c_3[-2r_1 - r_2 + r_4 + 2r_5] \\ = c_0[s_1 + s_2 + s_3 + s_4 + s_5] + c_1[-2s_1 - s_2 + s_4 + 2s_5] \\ + c_2[4s_1 + s_2 + s_4 + 4s_5] + c_3[-8s_1 - s_2 + s_4 + 8s_5] \end{aligned} \quad (8)$$

Hence, the schemes in this set should fulfill the following equations:

$$\begin{aligned} [s_1 + s_2 + s_3 + s_4 + s_5] &= 0 \\ [-2s_1 - s_2 + s_4 + 2s_5] &= 0 \\ 2[r_1 + r_2 + 1 + r_4 + r_5] &= [4s_1 + s_2 + s_4 + 4s_5] \\ 6[-2r_1 - r_2 + r_4 + 2r_5] &= [-8s_1 - s_2 + s_4 + 8s_5] \end{aligned} \quad (9)$$

Table 2: Set of second derivative approximations of order 4

Schemes	r_1	r_2	r_4	r_5	s_1	s_2	s_3	s_4	s_5
SDO4-1	$\frac{1}{13}$	$-\frac{2}{13}$	0	0	0	$\frac{12}{13}$	$-\frac{24}{13}$	$\frac{12}{13}$	0
SDO4-2	$\frac{1}{33}$	0	$\frac{2}{33}$	0	0	$\frac{12}{11}$	$-\frac{24}{11}$	$\frac{12}{11}$	0
SDO4-3	0	$\frac{2}{33}$	0	$\frac{1}{33}$	0	$\frac{12}{11}$	$-\frac{24}{11}$	$\frac{12}{11}$	0
SDO4-4	0	0	$-\frac{2}{13}$	$\frac{1}{13}$	0	$\frac{12}{13}$	$-\frac{24}{13}$	$\frac{12}{13}$	0
SDO4-5	0	-1	0	0	-1	3	-3	1	0
SDO4-6	$\frac{1}{11}$	0	0	0	$\frac{2}{11}$	$\frac{6}{11}$	$-\frac{18}{11}$	$\frac{10}{11}$	0
SDO4-7	0	0	$\frac{1}{11}$	0	$-\frac{1}{11}$	$\frac{15}{11}$	$-\frac{27}{11}$	$\frac{13}{11}$	0
SDO4-8	$\frac{1}{35}$	0	0	0	$-\frac{2}{35}$	$\frac{6}{5}$	$-\frac{78}{35}$	$\frac{38}{35}$	0
SDO4-9	$\frac{13}{37}$	$-\frac{38}{37}$	0	0	0	0	$\frac{12}{37}$	$-\frac{24}{37}$	$\frac{12}{37}$
SDO4-10	$-\frac{1}{3}$	0	$-\frac{38}{3}$	0	0	0	-12	24	-12
SDO4-11	$-\frac{5}{34}$	0	0	$\frac{19}{34}$	0	0	$\frac{24}{17}$	$-\frac{48}{17}$	$\frac{24}{17}$
SDO4-12	0	$-\frac{1}{2}$	$-\frac{13}{2}$	0	0	0	-6	12	-6
SDO4-13	0	$-\frac{10}{33}$	0	$\frac{13}{33}$	0	0	$\frac{12}{11}$	$-\frac{24}{11}$	$\frac{12}{11}$
SDO4-14	0	$\frac{1}{11}$	0	0	0	$\frac{13}{11}$	$-\frac{27}{11}$	$\frac{15}{11}$	$-\frac{1}{11}$
SDO4-15	$\frac{1}{35}$	0	0	0	0	$\frac{38}{35}$	$-\frac{78}{35}$	$\frac{6}{5}$	$-\frac{2}{35}$
SDO4-16	0	0	-1	0	0	1	-3	3	-1
SDO4-17	0	0	0	$\frac{1}{11}$	0	$\frac{10}{11}$	$-\frac{18}{11}$	$\frac{6}{11}$	$\frac{2}{11}$

2.3. Set of second derivative approximations of order 5:

In this part, five order schemes for the second derivative are provided as introduced in Table 3. To establish this set of approximations for the second derivative, c_4 in Eq.(4) should not be zero and c_5, \dots, c_N are all zeros. From Eq.(4), it follows:

$$2c_2[r_1 + r_2 + 1 + r_4 + r_5] + 6c_3[-2r_1 - r_2 + r_4 + 2r_5] + 12c_4[4r_1 + r_2 + r_4 + 4r_5] = c_0[s_1 + s_2 + s_3 + s_4 + s_5] + c_1[-2s_1 - s_2 + s_4 + 2s_5] + c_2[4s_1 + s_2 + s_4 + 4s_5] + c_3[-8s_1 - s_2 + s_4 + 8s_5] + c_4[16s_1 + s_2 + s_4 + 16s_5] \quad (10)$$

Hence,

$$\begin{aligned}
 [s_1 + s_2 + s_3 + s_4 + s_5] &= 0 \\
 [-2s_1 - s_2 + s_4 + 2s_5] &= 0 \\
 2[r_1 + r_2 + 1 + r_4 + r_5] &= [4s_1 + s_2 + s_4 + 4s_5] \\
 6[-2r_1 - r_2 + r_4 + 2r_5] &= [-8s_1 - s_2 + s_4 + 8s_5] \\
 12[4r_1 + r_2 + r_4 + 4r_5] &= [16s_1 + s_2 + s_4 + 16s_5]
 \end{aligned}
 \tag{11}$$

Table 3: Set of second derivative approximations of order 5.

Schemes	r ₁	r ₂	r ₄	r ₅	s ₁	s ₂	s ₃	s ₄	s ₅
SDO5-1	0	$\frac{1}{10}$	$\frac{1}{10}$	0	0	$\frac{6}{5}$	$-\frac{12}{5}$	$\frac{6}{5}$	0
SDO5-2	$\frac{1}{46}$	0	0	$\frac{1}{46}$	0	$\frac{24}{23}$	$-\frac{48}{23}$	$\frac{24}{23}$	0
SDO5-3	1	10	0	0	12	-24	12	0	0
SDO5-4	$-\frac{1}{99}$	0	0	$\frac{10}{99}$	$-\frac{4}{33}$	$\frac{16}{11}$	$-\frac{28}{11}$	$\frac{40}{33}$	0
SDO5-5	0	$-\frac{2}{9}$	0	$\frac{1}{45}$	$-\frac{4}{15}$	$\frac{8}{5}$	$-\frac{12}{5}$	$\frac{16}{15}$	0
SDO5-6	0	0	$\frac{2}{29}$	$\frac{1}{145}$	$-\frac{12}{145}$	$\frac{192}{145}$	$-\frac{12}{5}$	$\frac{168}{145}$	0
SDO5-7	0	0	10	1	0	0	12	-24	12
SDO5-8	$\frac{1}{5}$	$-\frac{4}{5}$	$-\frac{14}{5}$	0	0	$-\frac{12}{5}$	$\frac{24}{5}$	$-\frac{12}{5}$	0
SDO5-9	$\frac{5}{32}$	$-\frac{5}{8}$	0	$\frac{7}{32}$	0	$\frac{3}{4}$	$-\frac{3}{2}$	$\frac{3}{4}$	0
SDO5-10	$\frac{1}{145}$	$\frac{2}{29}$	0	0	0	$\frac{168}{145}$	$-\frac{12}{5}$	$\frac{192}{145}$	$-\frac{12}{145}$

2.4. Set of second derivative approximations of order 6:

In this section, second derivative compact schemes of order six are introduced as shown in Table 4 . To obtain this set of approximations for the second derivative, c_5 in Eq.(4) should not be zero and c_6, \dots, c_N are all zeros. From Eq.(10), and it follows:

$$\begin{aligned}
 &2c_2[r_1 + r_2 + 1 + r_4 + r_5] + 6c_3[-2r_1 - r_2 + r_4 + 2r_5] + 12c_4[4r_1 + r_2 + r_4 + 4r_5] + \\
 &20c_5[-8r_1 - r_2 + r_4 + 8r_5] + \sum_{t=6}^N t(t-1)c_t[r_1(-2)^{t-2} + r_2(-1)^{t-2} + r_4(1)^{t-2} + \\
 &r_5(2)^{t-2}] = c_0[s_1 + s_2 + s_3 + s_4 + s_5] + c_1[-2s_1 - s_2 + s_4 + 2s_5] + c_2[4s_1 + s_2 + s_4 + \\
 &4s_5] + c_3[-8s_1 - s_2 + s_4 + 8s_5] + c_4[16s_1 + s_2 + s_4 + 16s_5] + c_5[-32s_1 - s_2 + s_4 + \\
 &32s_5] + \sum_{t=6}^N c_t[s_1(-2)^t + s_2(-1)^t + s_4(1)^t + s_5(2)^t] \tag{12}
 \end{aligned}$$

Therefore,

$$\begin{aligned}
 [s_1 + s_2 + s_3 + s_4 + s_5] &= 0 \\
 [-2s_1 - s_2 + s_4 + 2s_5] &= 0 \\
 2[r_1 + r_2 + 1 + r_4 + r_5] &= [4s_1 + s_2 + s_4 + 4s_5] \\
 6[-2r_1 - r_2 + r_4 + 2r_5] &= [-8s_1 - s_2 + s_4 + 8s_5] \\
 12[4r_1 + r_2 + r_4 + 4r_5] &= [16s_1 + s_2 + s_4 + 16s_5] \\
 20[-8r_1 - r_2 + r_4 + 8r_5] &= [-32s_1 - s_2 + s_4 + 32s_5]
 \end{aligned}
 \tag{13}$$

Table 4: Set of second derivative approximations of order 6.

Schemes	r ₁	r ₂	r ₄	r ₅	s ₁	s ₂	s ₃	s ₄	s ₅
SDO6-1	$-\frac{1}{9}$	-1	$\frac{1}{9}$	0	$-\frac{4}{3}$	4	-4	$\frac{4}{3}$	0
SDO6-2	0	$\frac{33}{185}$	$\frac{23}{185}$	$-\frac{1}{185}$	$\frac{12}{185}$	$\frac{204}{185}$	$-\frac{12}{5}$	$\frac{228}{185}$	0
SDO6-3	$-\frac{23}{22}$	$-\frac{120}{11}$	0	$\frac{1}{22}$	$-\frac{144}{11}$	$\frac{312}{11}$	$-\frac{192}{11}$	$\frac{24}{11}$	0
SDO6-4	$-\frac{11}{654}$	0	$\frac{40}{327}$	$-\frac{1}{218}$	$-\frac{16}{109}$	$\frac{168}{109}$	$-\frac{288}{109}$	$\frac{136}{109}$	0
SDO6-5	$-\frac{1}{14}$	$\frac{2}{7}$	$\frac{102}{7}$	$\frac{19}{14}$	0	$\frac{120}{7}$	$-\frac{240}{7}$	$\frac{120}{7}$	0
SDO6-6	0	$\frac{1}{9}$	-1	$-\frac{1}{9}$	0	$\frac{4}{3}$	-4	4	$-\frac{4}{3}$
SDO6-7	$-\frac{1}{185}$	$\frac{23}{185}$	$\frac{33}{185}$	0	0	$\frac{228}{185}$	$-\frac{12}{5}$	$\frac{204}{185}$	$\frac{12}{185}$

2.5. Set of second derivative approximations of order 7:

In this part, second derivative compact schemes of order seven are proposed as illustrated in Table 5. To obtain this set of approximations for the second derivative, c_6 in Eq.(5) should not be zero and c_7, \dots, c_N are all zeros. From Eq.(12), and it follows:

$$2c_2[r_1 + r_2 + 1 + r_4 + r_5] + 6c_3[-2r_1 - r_2 + r_4 + 2r_5] + 12c_4[4r_1 + r_2 + r_4 + 4r_5] + 20c_5[-8r_1 - r_2 + r_4 + 8r_5] + 30c_6[16r_1 + r_2 + r_4 + 16r_5] + \sum_{t=7}^N t(t - 1)c_t[r_1(-2)^{t-2} + r_2(-1)^{t-2} + r_4(1)^{t-2} + r_5(2)^{t-2}] = c_0[s_1 + s_2 + s_3 + s_4 + s_5] + c_1[-2s_1 - s_2 + s_4 + 2s_5] + c_2[4s_1 + s_2 + s_4 + 4s_5] + c_3[-8s_1 - s_2 + s_4 + 8s_5] + c_4[16s_1 + s_2 + s_4 + 16s_5] + c_5[-32s_1 - s_2 + s_4 + 32s_5] + c_6[64s_1 + s_2 + s_4 + 64s_5] + \sum_{t=7}^N c_t[s_1(-2)^t + s_2(-1)^t + s_4(1)^t + s_5(2)^t] \tag{14}$$

so,

$$\begin{aligned} [s_1 + s_2 + s_3 + s_4 + s_5] &= 0 \\ [-2s_1 - s_2 + s_4 + 2s_5] &= 0 \\ 2[r_1 + r_2 + 1 + r_4 + r_5] &= [4s_1 + s_2 + s_4 + 4s_5] \\ 6[-2r_1 - r_2 + r_4 + 2r_5] &= [-8s_1 - s_2 + s_4 + 8s_5] \\ 12[4r_1 + r_2 + r_4 + 4r_5] &= [16s_1 + s_2 + s_4 + 16s_5] \\ 20[-8r_1 - r_2 + r_4 + 8r_5] &= [-32s_1 - s_2 + s_4 + 32s_5] \\ 30[16r_1 + r_2 + r_4 + 16r_5] &= [64s_1 + s_2 + s_4 + 64s_5] \end{aligned} \tag{15}$$

Table 5: Set of second derivative approximation of order 7.

Schemes	r ₁	r ₂	r ₄	r ₅	s ₁	s ₂	s ₃	s ₄	s ₅
SDO7-1	$-\frac{1}{194}$	$\frac{12}{97}$	$\frac{12}{97}$	$-\frac{1}{194}$	0	$\frac{120}{97}$	$-\frac{240}{97}$	$\frac{120}{97}$	0

3. Order of Accuracy for the numerical schemes:

There are many ways of demonstrating the order of accuracy for the numerical schemes. one way is by calculating errors from solving problems with analytic solutions and finding the relations between these errors with different step sizes. Another approach is using a polynomial of order N :

$$T_N(x) = \sum_{t=0}^N c_t x^t$$

such that schemes of order k are exact for the polynomials of order k or less, and they usually have error terms for the polynomials of order greater than k .

3.1. Order of Accuracy to the Numerical schemes of order 3:

In this section, it can be proved that all third order compact finite difference approximations for f''_k are exact for the functions $T_3(x) = \sum_{t=0}^3 c_t x^t$ such that $c_3 \neq 0$ as follows :

Firstly, SDO3-1 can be expressed as: $f''_k = \frac{1}{h^2} [f_{k-1} - 2f_k + f_{k+1}]$. (16)

The left-hand side (LHS) of Eq. (16) is: $f''_k = 2c_2 + 6c_3x_k$,

while the RHS of Eq.(16) is: $\frac{1}{h^2} [f_{k-1} - 2f_k + f_{k+1}] = \frac{1}{h^2} [c_0 + c_1x_{k-1} + c_2x_{k-1}^2 + c_3x_{k-1}^3 - 2(c_0 + c_1x_k + c_2x_k^2 + c_3x_k^3) + c_0 + c_1x_{k+1} + c_2x_{k+1}^2 + c_3x_{k+1}^3]$

$$= \frac{1}{h^2} [c_1(x_{k-1} - 2x_k + x_{k+1}) + c_2(x_{k-1}^2 - 2x_k^2 + x_{k+1}^2) + c_3(x_{k-1}^3 - 2x_k^3 + x_{k+1}^3)]$$

$$= \frac{1}{h^2} [c_1(h - h) + c_2((x_k - h)^2 - 2x_k^2 + (x_k + h)^2) + c_3((x_k - h)^3 - 2x_k^3 + (x_k + h)^3)]$$

$$= \frac{1}{h^2} [2h^2c_2 + 6h^2c_3x_k] = 2c_2 + 6c_3x_k$$

Similarly, SDO3-2 can be written as: $-\frac{1}{2}f''_{k-1} + f''_k = \frac{1}{h^2} [\frac{1}{2}f_k - f_{k+1} + \frac{1}{2}f_{k+2}]$. (17)

The LHS of Eq.(17) is : $-\frac{1}{2}f''_{k-1} + f''_k = -\frac{1}{2}(2c_2 + 6c_3x_{k-1}) + 2c_2 + 6c_3x_k$
 $= c_2 + 3c_3(2x_k - x_{k-1}) = c_2 + 3c_3(x_k + h)$,

while the RHS of Eq.(17) is: $\frac{1}{h^2} [\frac{1}{2}f_k - f_{k+1} + \frac{1}{2}f_{k+2}] = \frac{1}{h^2} [\frac{1}{2}(c_0 + c_1x_k + c_2x_k^2 + c_3x_k^3) - (c_0 + c_1x_{k+1} + c_2x_{k+1}^2 + c_3x_{k+1}^3) + \frac{1}{2}(c_0 + c_1x_{k+2} + c_2x_{k+2}^2 + c_3x_{k+2}^3)]$

$$= \frac{1}{h^2} [c_1(\frac{1}{2}x_k - x_{k+1} + \frac{1}{2}x_{k+2}) + c_2(\frac{1}{2}x_k^2 - x_{k+1}^2 + \frac{1}{2}x_{k+2}^2) + c_3(\frac{1}{2}x_k^3 - x_{k+1}^3 + \frac{1}{2}x_{k+2}^3)]$$

$$= \frac{1}{h^2} [c_2(\frac{1}{2}x_k^2 - (x_k + h)^2 + \frac{1}{2}(x_k + 2h)^2) + c_3(\frac{1}{2}x_k^3 - (x_k + h)^3 + \frac{1}{2}(x_k + 2h)^3)]$$

$$= \frac{1}{h^2} [h^2c_2 + c_3(2h^2x_k + 3h^3)] = c_2 + 3c_3(x_k + h)$$

Also, SDO3-3 has the form: $-\frac{1}{3}f''_{k-2} + f''_k = \frac{2}{3h^2} [f_k - 2f_{k+1} + f_{k+2}]$. (18)

The LHS of Eq.(18) is : $-\frac{1}{3}f''_{k-2} + f''_k = -\frac{1}{3}(2c_2 + 6c_3x_{k-2}) + 2c_2 + 6c_3x_k = \frac{4}{3}c_2 + c_3(6x_k - 2x_{k-2})$

$$= \frac{4}{3}c_2 + c_3(6x_k - 2(x_k - 2h)) = \frac{4}{3}c_2 + 4c_3(x_k + h)$$

while the RHS of Eq.(18) is: $\frac{2}{3h^2} [f_k - 2f_{k+1} + f_{k+2}] = \frac{2}{3h^2} [c_0 + c_1x_k + c_2x_k^2 + c_3x_k^3 - 2(c_0 + c_1x_{k+1} + c_2x_{k+1}^2 + c_3x_{k+1}^3) + c_0 + c_1x_{k+2} + c_2x_{k+2}^2 + c_3x_{k+2}^3]$

$$= \frac{2}{3h^2} [c_1(x_k - 2x_{k+1} + x_{k+2}) + c_2(x_k^2 - 2x_{k+1}^2 + x_{k+2}^2) + c_3(x_k^3 - 2x_{k+1}^3 + x_{k+2}^3)]$$

$$= \frac{2}{3h^2} [c_2(x_k^2 - 2(x_k + h)^2 + (x_k + 2h)^2) + c_3(x_k^3 - 2(x_k + h)^3 + (x_k + 2h)^3)]$$

$$= \frac{2}{3h^2} [2h^2c_2 + c_3(6h^2x_k + 6h^3)] = \frac{4}{3}c_2 + 4c_3(x_k + h)$$

The last approximation in this set is SDO3-4, which can be given as:

$$f''_k + f''_{k+2} = \frac{2}{h^2} [f_{k-1} - 2f_k + f_{k+1}]. \quad (19)$$

The LHS of (19) is : $f_k'' + f_{k+2}'' = 2c_2 + 6c_3x_k + 2c_2 + 6c_3x_{k+2} = 4c_2 + 6c_3(x_k + x_{k+2})$
 $= 4c_2 + 6c_3(x_k + x_k + 2h) = 4c_2 + 12c_3(x_k + h),$

While the RHS of (19) is: $\frac{2}{h^2} [f_{k-1} - 2f_k + f_{k+1}] = \frac{2}{h^2} [(c_0 + c_1x_k + c_2x_k^2 + c_3x_k^3) - 2(c_0 + c_1x_{k+1} + c_2x_{k+1}^2 + c_3x_{k+1}^3) + (c_0 + c_1x_{k+2} + c_2x_{k+2}^2 + c_3x_{k+2}^3)]$
 $= \frac{2}{h^2} [c_1(x_k - 2x_{k+1} + x_{k+2}) + c_2(x_k^2 - 2x_{k+1}^2 + x_{k+2}^2) + c_3(x_k^3 - 2x_{k+1}^3 + x_{k+2}^3)]$
 $= \frac{2}{h^2} [c_2(x_k^2 - 2(x_k + h)^2 + (x_k + 2h)^2) + c_3(x_k^3 - 2(x_k + h)^3 + (x_k + 2h)^3)]$
 $= \frac{2}{h^2} [2h^2c_2 + c_3(6h^2x_k + 6h^3)] = 4c_2 + 12c_3(x_k + h)$

Now, the remaining terms or the error terms can be found when using polynomials of order higher than 3. Hence, $T_7(x)$ is used to get the coefficients of the remaining polynomials as it is illustrated in the table below:

TABLE 6: The coefficients of the remaining polynomials for the approximations of order 3.

Schemes	c ₀	c ₁	c ₂	c ₃	c ₄	c ₅	c ₆	c ₇
SDO3-1	0	0	0	0	-2	0	-2	0
SDO3-2	0	0	0	0	-13	-5	-46	-42
SDO3-3	0	0	0	0	$-\frac{76}{3}$	$\frac{100}{3}$	$-\frac{604}{3}$	364
SDO3-4	0	0	0	0	20	100	356	1092

3.2. Order of Accuracy to the Numerical schemes of order 4:

As in the previous section, the fourth order compact approximations for f''_k are exact for the function $T_4(x)$ such that $c_4 \neq 0$. Also, $T_8(x)$ is used to get the coefficients of the remaining polynomials as shown in the table below:

Table 7: The coefficients of remaining polynomials for the approximations of order 4

Schemes	c ₀	c ₁	c ₂	c ₃	c ₄	c ₅	c ₆	c ₇	c ₈
SDO4-1	0	0	0	0	0	$-\frac{120}{13}$	$\frac{396}{13}$	$-\frac{1260}{13}$	$\frac{3448}{13}$
SDO4-2	0	0	0	0	0	$-\frac{40}{11}$	$\frac{156}{11}$	$-\frac{420}{11}$	$\frac{1208}{11}$
SDO4-3	0	0	0	0	0	$\frac{40}{11}$	$\frac{156}{11}$	$\frac{420}{11}$	$\frac{1208}{11}$
SDO4-4	0	0	0	0	0	$\frac{120}{13}$	$\frac{396}{13}$	$\frac{1260}{13}$	$\frac{3448}{13}$
SDO4-5	0	0	0	0	0	-10	30	-84	196
SDO4-6	0	0	0	0	0	$-\frac{100}{11}$	$\frac{336}{11}$	$-\frac{1092}{11}$	$\frac{3056}{11}$
SDO4-7	0	0	0	0	0	$-\frac{10}{11}$	$\frac{66}{11}$	$-\frac{84}{11}$	$\frac{284}{11}$

SDO4-8	0	0	0	0	0	$\frac{100}{35}$	$\frac{528}{35}$	$\frac{1092}{35}$	$\frac{4016}{35}$
SDO4-9	0	0	0	0	0	$-\frac{1680}{37}$	$\frac{4356}{37}$	$\frac{17388}{37}$	$-\frac{41416}{37}$
SDO4-10	0	0	0	0	0	160	204	1428	1144
SDO4-11	0	0	0	0	0	$\frac{1200}{17}$	$\frac{1872}{17}$	$\frac{13104}{17}$	$\frac{18992}{17}$
SDO4-12	0	0	0	0	0	60	162	504	1132
SDO4-13	0	0	0	0	0	$\frac{400}{11}$	$\frac{1236}{11}$	$\frac{4452}{11}$	$\frac{12296}{11}$
SDO4-14	0	0	0	0	0	$\frac{10}{11}$	$\frac{66}{11}$	$\frac{84}{11}$	$\frac{284}{11}$
SDO4-15	0	0	0	0	0	$\frac{100}{35}$	$-\frac{528}{35}$	$\frac{1092}{35}$	$-\frac{4016}{35}$
SDO4-16	0	0	0	0	0	10	30	84	196
SDO4-17	0	0	0	0	0	$\frac{100}{11}$	$\frac{336}{11}$	$\frac{1092}{11}$	$\frac{3056}{11}$

3.3. Order of Accuracy to the Numerical schemes of order 5:

Additionally, the fifth order compact approximations for f''_k are exact for the function $T_5(x)$ such that $c_5 \neq 0$, and $T_8(x)$ is used to get the coefficients of the remaining polynomials as introduced in the table below:

Table 8: The coefficients of remaining polynomials for the approximations of order 5

Schemes	c_0	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8
SDO5-1	0	0	0	0	0	0	$\frac{18}{5}$	0	$\frac{44}{5}$
SDO5-2	0	0	0	0	0	0	$\frac{432}{23}$	0	$\frac{3536}{23}$
SDO5-3	0	0	0	0	0	0	36	-252	1096
SDO5-4	0	0	0	0	0	0	$\frac{36}{11}$	$\frac{28}{11}$	$-\frac{24}{11}$
SDO5-5	0	0	0	0	0	0	$\frac{92}{5}$	$\frac{28}{5}$	$\frac{664}{5}$
SDO5-6	0	0	0	0	0	0	$\frac{1188}{145}$	$\frac{252}{145}$	$\frac{6856}{145}$
SDO5-7	0	0	0	0	0	0	36	252	1096
SDO5-8	0	0	0	0	0	0	$\frac{684}{5}$	$-\frac{252}{5}$	$\frac{5624}{5}$
SDO5-9	0	0	0	0	0	0	$\frac{459}{4}$	$\frac{63}{4}$	$\frac{4474}{4}$
SDO5-10	0	0	0	0	0	0	$\frac{1188}{145}$	$-\frac{252}{145}$	$\frac{6856}{145}$

3.4. Order of Accuracy to the Numerical schemes of order 6:

Similarly, the sixth order compact approximations for f''_k are exact for the function $T_6(x)$ such that $c_6 \neq 0$. Also, $T_9(x)$ is used to get the coefficients of the remaining polynomials as shown in the table below:

Table 9: The coefficients of remaining polynomials for the approximations of order 6.

Schemes	c_0	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9
SDO6-1	0	0	0	0	0	0	0	28	-112	424
SDO6-2	0	0	0	0	0	0	0	$-\frac{252}{185}$	$-\frac{3952}{185}$	$-\frac{3816}{185}$
SDO6-3	0	0	0	0	0	0	0	$\frac{3024}{11}$	$-\frac{9616}{11}$	$\frac{45792}{11}$
SDO6-4	0	0	0	0	0	0	0	$\frac{336}{109}$	$-\frac{3824}{109}$	$\frac{5088}{109}$
SDO6-5	0	0	0	0	0	0	0	$\frac{4410}{4}$	$\frac{13300}{4}$	$\frac{66780}{4}$
SDO6-6	0	0	0	0	0	0	0	-28	-108	424
SDO6-7	0	0	0	0	0	0	0	$\frac{252}{185}$	$-\frac{3952}{185}$	$\frac{3816}{185}$

3.5. Order of Accuracy to the Numerical scheme of order 7:

Finally, the seventh order compact approximations for f''_k are exact for the function $T_7(x)$ such that $c_7 \neq 0$. Also, $T_9(x)$ is used to get the coefficients of the remaining polynomials as in the table below:

Table 7: The coefficients of remaining polynomial for the approximation of order 7

Scheme	c_0	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9
SDO7-1	0	0	0	0	0	0	0	0	$-\frac{2480}{97}$	0

4. Conclusion:

To obtain the second derivative approximation, many families of compact methods are proposed in this work according to some polynomials of different degrees. In addition, the construction methodology of deriving these families is introduced in clear and simple way. As shown in tables, all schemes in each family have the same order of accuracy, which is verified by obtaining the coefficients of remaining polynomial. From the results, the characteristics of each approximation are clearly shown, so they can be applicable to solve problems from Computational Fluid Dynamics (CFD) like one or two-dimensional convection–diffusion equation. For the future work, the proposed method can be generalized to construct schemes for high derivatives as needed in providing accurate and stable solutions.

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